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From cases to general principles: A call for theory development through agent-based modeling

Abstract

Virtually all current major social and environmental challenges such as financial crises, migration, the erosion of democratic institutions, and the loss of biodiversity involve complex systems comprising decision-making, interacting, adaptive agents. To understand how such agent-based complex systems function and respond to change and disturbances, agent-based modeling (ABM) is increasingly recognized as the main way forward. Many motivating examples of agent-based models exist that are realistic enough to successfully support the management of complex systems, but these solutions are case-specific and contribute few general insights into the functioning of systems. General theory, though, is highly needed because we cannot model each system and question. Still, across disciplines, a critical mass of expertise has accumulated that could transform ABM into a more coherent and efficient approach to discover the functioning of complex social-economic-ecological systems. To this end, we need a cross-disciplinary discussion among researchers and a goal-oriented synthesis to identify the general principles and theories essential to improve our understanding and management of complex systems.

MOTIVATION

We live in networks (Lazer et al., 2009) where individual actions and institutional policies may have unintended consequences that are hard to oversee or even predict. Digitalization and information technology link different areas so that "*systems that used to be separate are now interconnected and interdependent*" (Sargut and McGrath, 2011, p. 70). Analyzing, understanding, predicting, and managing the dynamics of these agent-based complex systems (ACSs) are some of the most urgent issues these days (Sargut and McGrath, 2011).

To understand how such systems function and respond to environmental changes and disturbances, agent-based modeling (ABM; also called individual-based modeling, IBM) is increasingly recognized as the main way forward (Macal, 2016, Law, 2015). The approach captures dynamics that arise from the behavior and interactions of individual agents, such as bird flocking behavior and the S-shaped diffusion process of innovations in markets resulting from individual consumer adoption decisions (Schubring et al., 2016, Garcia and Jager, 2011). ABM allows for a holistic view by linking different levels of an organization (Gräbner, 2016, p.245). For example, agent-based models describing the complex socioeconomic dynamics of land use at multiple levels are suitable to explore the particular impacts of environmental settings on the mitigation and adaptation strategies of humans or organizations to climate change (Balbi and Giupponi, 2009). By performing simulation experiments, explanations of complex developments can be found that are too complex to oversee otherwise. This may also include the consideration of rare or improbable events, to be better prepared for the future. Consequently, ABM is of increasing relevance and we find applications in virtually all research fields where adaptive agents matter, such as socio-ecology (Balbi and Giupponi, 2009, DeAngelis and Mooij, 2005a, Tesfatsion, 2002), economics (Tesfatsion, 2002), management (Kiesling et al., 2012), geography (Heppenstall et al., 2011, Crooks and Heppenstall, 2012), and ecology (Railsback and Johnson, 2011).

Notwithstanding the relevance of understanding ACSs and the value of ABM for accomplishing this goal, the method seems stuck in a stage of ad hoc model development and exploration. Besides all the merits of ABM applications, scientific progress in ABM has been slower than expected, which was poignantly described by Nobel laureate Paul Krugman as follows: "*I was one of the people who got all excited about the possibility of getting somewhere with very detailed agent-based models — but* *that was 20 years ago. And after all this time, it's all still manifestos and promises of great things one of these days*" (Krugman, 2010).

The majority of existing agent-based models focus on specific systems, which limits their generality. The scientific community recognizes this more and more, and the current situation has been described recently as the "*yet another model syndrome*" (O'Sullivan et al., 2016), presenting model after model without accumulating general theoretical insights into systems and their dynamics. As a consequence, there is a "call for theoretical engagement" (O'Sullivan et al., 2016, p.184), and it is the aim of this paper to open a dialog on theory development through ABM.

We claim that to cope with the challenges of modern complex and highly interconnected ACSs, we have to complement the current focus on single cases with a second perspective regarding the identification of more general principles. At the system level, we need to identify and understand the general principles, such as ACSs' self-organization, their ability to cope with change and stress (resilience), and their propensity toward catastrophic, sudden changes (regime shifts, Egli et al., 2018). Similarly, there is a need to more systematically accumulate knowledge at the level of individual behaviors in the form of, say, reusable, generic submodules of agents. For this purpose, we need tested, well-understood, and modular building blocks that are ready to implement in the agent-based models of specific ACSs. This would increase credibility and allow for systematic learning beyond the respective case, which in the end improves the predictive capabilities of our models.

REASONS FOR THE CURRENT SITUATION

We see at least three possible reasons why this has not been achieved so far. First, it might paradoxically result from a key benefit of ABM, namely its flexibility and ability to embrace complexity. This involves many degrees of freedom in the modeling process. Keeping such agent-based models at a generic level, for example by trying to model "pastoralist systems" in general, would leave room for so many possible outcomes that the model would be of little use for practical purposes. Such generic agent-based models exist, for example on opinion dynamics, cultural dissemination, and segregation, but it remains unclear how well they capture the organization of real systems.

To avoid this, ABM developers that strive for inferences about the real world relate their modeling efforts to specific empirical cases, which is reflected in an increasing number of empirically validated and calibrated models (Stillman et al., 2015). This research strategy narrows the degrees of freedom in model parameters and structure, which leads to testable predictions and management recommendations for the modeled system. The price for this is a loss of generality, both because a specific system is modeled and because the focus on this system and robust predictions seem to prevent most ABM developers from thinking about general principles, or theories, that go beyond their specific case.

Second, ABM is a sophisticated research tool, which comes with its methodological challenges. Due to the inherent complexity of many agent-based models, there are concerns about their internal validity (Lehtinen and Kuorikoski, 2007, p.323) and our ability to understand these models. This skepticism has been expressed by Roughgarden (2012, p.8): "*With simulation it may be impossible to drill down to what assumptions are responsible for conclusions, to discern the causal connections between initial conditions and results, and simulation invites unsophisticated and sloppy research together with naive hocus-pocus about the magic of emergence.*" In many disciplines, an exclusive link between the analytical tractability of models and theory is taken for granted (Evans et al., 2013). In particular, economics endorses analytical solutions as a necessary precondition for contributions to theory (Lehtinen and Kuorikoski, 2007), although it often requires an oversimplification of the described processes, hindering its suitability to tackle most problems of complex systems. ABM provides a new avenue to model interdependencies and processes in algorithmic structures, which gives the theory-generating process a new appearance. The specifics of the method and the new methodological challenges that follow from this, however, have slowed theory development so far.

Third, it might take time for a complex approach such as ABM to mature. Calculus or statistics were not developed in just a few decades. In ecology, which has the longest history of using agent-based models (Vincenot, 2018), such models are now accepted as a tool for tackling applied problems, but not for identifying general principles or developing a general theory (Evans et al., 2013). There are indeed indicators of the methodological maturation of ABM, including topics such as standardized communication, validation, and sensitivity analysis (Grimm and Berger, 2016b, Hauke et al., 2017, Schulze et al., 2017). These tentative explanations of the current situation are not exclusive and have to be explored further if we want to make ABM suitable for much-needed theory development.

THEORY DEVELOPMENT THROUGH ABM

There is still little awareness of the need for a more general theory in ABM, or such a theory is considered to be impossible to achieve with this approach. Theories explain reoccurring patterns (also referred to as stylized facts, signals, or regularities) and describe how the system in question is internally organized. Computational modeling is the next level of theory development that allows for the formalization of interactions and adaptation processes. Further, ABM can combine multiple approaches and go side by side with mathematical models by including probability functions or logical rules in submodels.

In particular, we seek two kinds of theories: theories addressing the system and theories addressing the behavior of agents. The first perspective aims to identify patterns at the system level to understand the underlying organization of ACSs. From the second perspective, we include alternative submodels of agent behavior to analyze the macro-response at the system level. Ultimately, these two kinds of theories need to be matched to each other because the behavior of agents and system-level features are inseparably linked. Agent-based theory development is thus cross-level. This is in contrast to theory in many other fields. For example, theory in community ecology ignores behavior, whereas theory in classical behavioral ecology ignores feedback at higher organizational levels.

For some systems, cross-level theory development through ABM has already worked well (e.g., models explaining the emergence of fish schools and bird flocks). The latter started by assuming that fixed distances determine behavior before realizing that real birds in fact take six to eight neighbors into account. Finally, they managed to reproduce observed patterns by also including the basic principles of flight physics (e.g., Hemelrijk and Hildenbrandt 2015). Similarly, theory development should also be the aim of ABM, linking behavior to the observed patterns of systems where the behavioral context is more comple x than in bird flocks.

Another good example of theory development through ABM is the study by Martin et al. (2013). This simulation study shows how one generic theory, namely Dynamic Energy Budget theory, can be used to extrapolate the effect of toxicants measured at the individual level to effects on population dynamics. This study reproduces the population density by one food level. Beyond this, the results showed the density and size distribution of multiple food levels and toxicant exposure, which was not seen before. This study also provides a good example of how circularity can be avoided, as it produces new predictions.

Empirical knowledge is an important source of patterns and candidate submodels of behavior. Experts can also be the first to formulate a hypothesis on why certain things happen. Likewise, the stakeholders' perspective helps asking relevant questions about a system and thereby developing theory that is related to real world problems. Within the limits of the formalized system, we may, using ABM and theory development, achieve a deep understanding of interdependencies and process trajectories that would be hard to obtain otherwise. The theory supports a coherent understanding of complex systems, thus explicating their relevant features in a systematic way. Alternative approaches, based on highly stylized representations, are less likely to lead to testable theories because they rather demonstrate certain concepts or ideas than real systems. Models based on opinion dynamics in social sciences and Lotka-Volterra models in ecology are prominent examples.

ABM has some challenges that are similar to those of other modeling approaches. ACSs are not always self-defined, but we have to define their boundaries, which is not often easy. We think that the formalization of a defined system by one valid model may produce hypotheses of patterns suitable to represent a particular system. This can be done, for example, by robustness analyses (Grimm and Berger 2016a) and even extended sensitivity analyses. To achieve generality, however, we would ideally focus on generic patterns that define classes of systems, not only specific ones, for example tree/grass coexistence in savannas. It is important, though, to go beyond single patterns and try to reproduce entire sets of patterns ("pattern-oriented modeling"; Grimm and Railsback 2010).

Theory development with agent-based models also needs to consider the algorithmic nature of ACSs. These systems are driven by context-dependent and stochastic events such as natural selection and the life history of individuals (Dennett and Mittwoch, 1996). Although aspects of ACSs may be captured by mathematical models that are analytically tractable, algorithmic representations provided by ABM might be more adequate for many purposes. In ecology, this already leads to standard algorithms in certain ecological settings; see, for example, the zone-of-influence approach for the description of local interactions among plants (Weiner et al., 2001, Berger et al., 2008). Moreover, to represent home range behavior or territorial dynamics, we do not need a new approach in every single model; rather, we can build on existing models, which are based either on maps of habitat quality (e.g., Wang and Grimm, 2007, Carter et al., 2014) or on tracking data and the assumption that animals remember good places (e.g., Nabe-Nielsen et al., 2018).

Taking such an algorithmic perspective involves further challenges, which have to be handled. First, it requires a more intensive cultivation of the skill of computational thinking, such as the algorithmic problem-solving and abstraction techniques developed by computer scientists (Wing, 2006). Second, as already indicated above, it might also change the role of mathematics and simulation with respect to theory development. Theories about ACSs that cannot be expressed mathematically can be represented algorithmically. To allow for generalizations, a possible contribution of mathematics could be then to formulate a theory of algorithms. In terms of culture, this could affect the different traditions in ecology, economics, and the other social sciences (e.g., how mathematics and computer simulations are applied and relate to each other). Answers to these challenges emerge, but are distributed among many disciplines and have to be incorporated.

NEXT STEPS

How to move forward? First, each agent-based modeler can contribute more to theory development by referring, as required in the ODD (Overview, Design concepts, Details) protocol's design concept of "basic principles" (Grimm et al., 2010, Grimm et al., 2006), to the general theories and concepts that guide the design of the model and by explicitly discussing the model's results in terms of these theories. Did they work? Were they useful? Did they need to be refined within the agent-based model? Why?

Also the fact that systems often depict stable patterns (also referred to as stylized facts) could be a possible way forward. First, there could be some general mechanism creating them. If these patterns are similar for different systems (even among classes of systems), this might provide further possible avenues for theory development. Second, these patterns might contain information that can provide insights into the general working of the system or the process under investigation.

In addition, we need methods and approaches that support the theory development process in ABM. Some approaches already exist that may improve the specification and analysis of models in this regard. To focus on both theory and application, we need to force "*cloudy areas to be addressed in clear specification*" (Harrison et al., 2007, p.1233). The ODD protocol for model specification supports this process (Grimm et al., 2010, Grimm et al., 2006). Systematic designs of experiments support the analysis of simulation models to draw valid and reliable conclusions from simulation results (Lorscheid et al., 2012, Lorscheid and Meyer, 2016). All these approaches can contribute to improving the rigor of agent-based models and offer systematic ways for valid theory development by ABM.

In addition, various ways of theory development have been suggested, including pattern-oriented theory development (Grimm and Railsback, 2012, Railsback and Harvey, 2013), breaking models (Thiele and Grimm, 2015), and robustness analysis (Grimm and Berger, 2016a). Management research and sociology have developed strategies on how to derive theory from single or multiple case studies. The principles of "pattern-oriented modeling" and stylized facts, for example, can be of added value to focus on and evaluate the core mechanics of a model (Grimm et al., 2005, Meyer, 2019, Heine et al., 2005). Unfortunately, these methods have never been sufficiently considered or discussed across the disciplinary boundaries, nor combined in an overall, systematic research strategy. This discussion, however, is necessary. ABM researchers need to develop concrete roadmaps and practical guidelines to open ways for more coherent and rigorous research that, in the long run, also leads to a better acceptance of agent-based theory.

This quest for theory also poses the question of how to organize our collective learning and gather best practices. How can we accumulate knowledge more systematically from our model-based analyses of ACSs? Systematic reviews of existing agent-based models with respect to their core mechanisms would allow us to identify similarities and differences in the investigated cases. A set of the typical patterns/stylized facts of different classes of ACSs might also be used as a coordinating device for modeling efforts (Meyer, 2011, Heine et al., 2005). As Hilbert's problems set a challenge for mathematics, explaining the patterns observed regularly for certain ACSs may set the path for a community of modelers in a domain. Both efforts might lead to better knowledge of the underlying organization of ACSs.

Given the general character of these questions, the epistemological perspective is also critical but often ignored by the community of ABM developers. It is important to keep in mind that "theory" has multiple meanings, ranging from the colloquial interpretation as speculative guess, or conjecture, to its interpretation in physics as an explanation of observed phenomena that have been well confirmed by testing the theory's predictions. What kinds of predictions can we expect or should we aim for with agent-based models? Should we seek theory rather at the level of the agent's behavior or is it also possible at the entire system level?

CONCLUSION

This paper cannot depict a fully developed solution, but wants to open the dialog concerning the posed problem and possible ways out. Without such a general quest for theory development, ABM will continue delivering patchwork results, which is insufficient to meet the grand societal and environmental challenges in our interconnected and fast-changing world. Instead of developing agent-based models for each question and system, we need to identify robust principles that allow both individuals and policymakers to make the right decisions. This is a call towards a general, cross-level, and cross-disciplinary theoretical engagement concerning ACSs. Following the "*call for theoretical engagement*" (O'Sullivan et al., 2016, p. 184), the modeling community needs:

1. To gain a **better understanding of how to use ABM to derive the general principles** of the complex systems we live in. For this, we need a cross-disciplinary discussion and a goal-oriented synthesis to transform ABM into a more coherent, efficient approach to identify general principles and theories.
2. A **compilation and critical reflection of existing methods and best practice in ABM research** fostering the development and dissemination of standards. This also requires a discussion of the existing gaps and obstacles for successful theory development through ABM including a philosophical discussion on whether ABM extends classical theory to more complex situations or represents a radically new research program (DeAngelis and Mooij, 2005b).
3. To **formulate a roadmap** to overcome current obstacles to use the potential of ABM as a powerful and much-needed approach for theory development.

The main purpose of this call is to create awareness of these challenges. We invite peers in all disciplines using ABM to relate their more or less case-specific work to theory and consider theory development to be an integral part of even the most applied ABM. If we all force ourselves to include in all our ABM publications at least one paragraph in the discussion addressing the question "What have we learned in terms or general theory?", we would already contribute to this first important step.

We invite complementary or opposing views to those expressed by us, and we hope to instigate a much-needed discussion on theory development among agent-based modelers, which hopefully will result in explicit articles, special issues, and projects. We ourselves are organizing a series of three workshops entitled "From cases to general principles: Theory development through agent-based modeling"[1]. These symposia will provide a platform to connect modelers from different disciplines and epistemologists for critical reflections and the collection of best practices.

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[1] The events will take place in Hanover, Germany in 2018–2020. For the website on this initiative, see www.abm-theory.org.

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